1-Hexanol

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 1.92

Global applicability domain: Inside

Local applicability domain index: 7.21e-01

Confidence level: 8.25e-01

Nearest Neighbors from the Training Set

Image not found	Image not found	Image not found
1-Hexanol	1-Heptanol	Isopentyl alcohol
Measured: 2.03	**Measured:** 2.62	**Measured:** 1.16
Predicted: 1.92	**Predicted:** 2.53	**Predicted:** 1.24